The effect of bulk composition on the behavior of sulfur during core formation. H. L. Bercovici[1], L. T. Elkins-Tanton[1], L. Schaefer[2], [1]School of Earth and Space Exploration, Arizona State University, Tempe, AZ 85282 (hbercovi@asu.edu), [2]Stanford University, Stanford, CA 94305.

Introduction: While many studies have looked at sulfur partitioning in large planets [e.g., 1, 2] and the effect of sulfur on the partitioning behavior of other elements [e.g., 3, 4], few have examined how sulfur partitions in planetesimals. Evidence from trace elements in iron meteorites, some of which represent fragments of early planetesimals' cores, suggests that sulfur was present in varying amounts [3]. As sulfur would alter the geochemical and physical evolution of a planet's core as it fractionates [4], we present a model that determines how the parent body's bulk composition, and therefore oxygen fugacity, effects sulfur partitioning during differentiation.

Iron meteorites and sulfur: Trace elements (TE) in iron meteorites follow a trend that suggests sulfur plays a major role in a core's geochemical evolution. For example, germanium (Ge) has both chalcophile and siderophile tendencies, while gold (Au) is only siderophile [3]. If no sulfur were present in a core, Ge and Au plotted together would produce a linear relationship. However, Ge vs. Au does not produce a linear trend in most iron meteorites, implying sulfur was present in the cores during fractionation [3].

In contrast to the TE trends, sulfur is not measured in geochemical analyses of iron meteorites except in non-homogeneously distributed triolite nodules [3]. Some studies propose that sulfur forms an immiscible S-rich liquid that separates from metal components in an iron core, especially at low pressures [3]. The amount of sulfur required to form an immiscible liquid in a core varies, but can be as low as 5 wt.% S in the presence of phosphorus [5]. A S-rich liquid is less dense than Fe-Ni liquid or crystals [3], and could float to the core-mantle boundary or, under the right conditions, erupt onto the surface of an exposed core. Either case could explain the lack of sulfur in iron meteorites.

(16) Psyche and sulfur: This study is also pertinent to the 2022 NASA mission to Psyche, the largest metallic body in the asteroid belt. The asteroid is hypothesized to be the core of a stripped planetesimal. The core would have been separated from the rest of the planetary body during collisions from other celestial bodies [6].

We would like to apply this model to Psyche and determine how much sulfur the asteroid could potentially contain, which would change the geochemical and physical evolution of the asteroid [4]. We also want to understand if an immiscible S-rich fluid could potentially form, later flooding the surface of Psyche due its high buoyancy [3]. The amount of sulfur in Psyche would affect what the spacecraft measures when it arrives in 2026.

Sulfur partitioning model: We investigate sulfur partitioning into a metal core during primary differentiation in a planetesimal the size of Vesta (r=~263 km [4]). We focus on determining how the parent body's bulk composition, and oxygen fugacity (f_{O2}), control sulfur's partition coefficient (D_S), and thus the core's final composition.

Finding D_S*:* We assume the planetesimal is entirely molten due to ^{26}Al, and sulfur partitions between the core and mantle according to $D_S = \frac{X_S^{core}}{X_S^{mantle}}$, where X_S^{core} is the moles of sulfur in the core and X_S^{mantle} is the moles of sulfur in the mantle [1, 2]. We used the following equation to find D_S [2]: $log\, Ds = a + \frac{b}{T} + c\left(\frac{P}{T}\right) + log\, X_{FeO}^{mantle} - log C_s + d log(1 - X_O^{core})$, where *a, b, c,* and *d* are constants derived experimentally, *T* is temperature in K, which ranges from 1875-2175 K in order to ensure complete melting [2], *P* is pressure in GPa and held constant at 1 GPa, X_{FeO}^{mantle} is the mole fraction of FeO in the silicate mantle, C_S is the sulfide capacity of the mantle, and X_O^{core} is the mole fraction of oxygen in the core during accretion, which is assumed to be 0 for a planetesimal. We calculate *Cs* with the equation [1]: $log C_S = -5.705 + 3.15X_{FeO}^{mantle} + 2.65X_{CaO}^{mantle} + 0.12X_{MgO}^{mantle} + 0.77X_{TiO_2}^{mantle} + 0.75(X_{Na_2O}^{mantle} + X_{K_2O}^{mantle})$, where X_M^{mantle} is the mole fraction of oxide M in the silicate mantle. The pressures used to experimentally determine the pressure partition coefficients for D_S and C_S are much higher (2-91 GPa [1, 2]) than what we would expect for a planetesimal (~1 GPa [4]). More experiments need to be done to determine sulfur's pressure partition coefficients at low pressures.

We use a range of bulk starting compositions; ordinary chondrites (H, L, LL), or OC, represent a

Table 1. *Bulk compositions of troilite (FeS), metallic iron (Fe), and oxidized iron (FeO) for different chondrite types [8].*

Chondrite Type	*H*	*L*	*LL*	*CI*	*CM*	*CO*	*CV*	*CK*
Bulk FeS (wt.%)	5.22	5.68	5.12	9.08	7.06	5.22	2.55	2.90
Bulk Fe (wt.%)	13.2	6.20	2.53	0	0.030	2.27	0.692	2.07
Bulk FeO (wt.%)	12.9	15.3	17.6	16.8	22.8	24.3	17.0	25.5

reduced parent body and carbonaceous chondrites (CI, CM, CO, CV, CK), or CC, represent an oxidized parent body [3, 7, 8]. Troilite is assumed to be the source of sulfur (Table 1).

Finding S in the core: We first determined the mole fraction of sulfur in the core using this relation [2]: $X_S^{core} = D_S * \left(\frac{X_S^{PB}}{D_S * n_{core} + n_{mantle}}\right)$, where X_S^{PB} is the molar fraction of sulfur in the parent body, and n_{core} and n_{mantle} are the total moles in the core and mantle, respectively, not including sulfur. We then found the mass of sulfur in the core after differentiation: $M_S^{core} = X_S^{core} * n_{core} * 32.06$. Lastly, we found the wt.% of sulfur in the core, $F_S^{core} = \frac{M_S^{core}}{M_{Fe}^{PB} + M_{Ni}^{PB} + M_S^{core}} * 100$, where M_{Fe}^{PB} and M_{Ni}^{PB} are the mass of nickel and iron in the bulk chondrite respectively and they are assumed to partition entirely into the core.

Results: Distribution coefficients are affected by temperature, initial bulk composition, and f_{O2}. Ordinary chondrite parent bodies have higher D_S values than CC bodies. Oxygen fugacity is the primary control that separates the chondritic bulk compositions graphed in Figure 1.

Similar to D_S values, f_{O2} is the primary controller separating the different parent body types graphed in Figure 2, but in the opposite manner. The oxidized parent bodies (CC) tend to have more sulfur in their cores than in reduced parent bodies (OC). The CI chondrites have the most S-rich core, while the H-chondrites produce the least S-rich core.

The sulfur present in the core is consistent with the amount of Fe and FeS in the chondrites (Table 1). H-chondrites contain the most reduced iron (Fe^0), and create a predominately metal iron core, even with later additions of sulfur. Conversely, CI chondrites contain

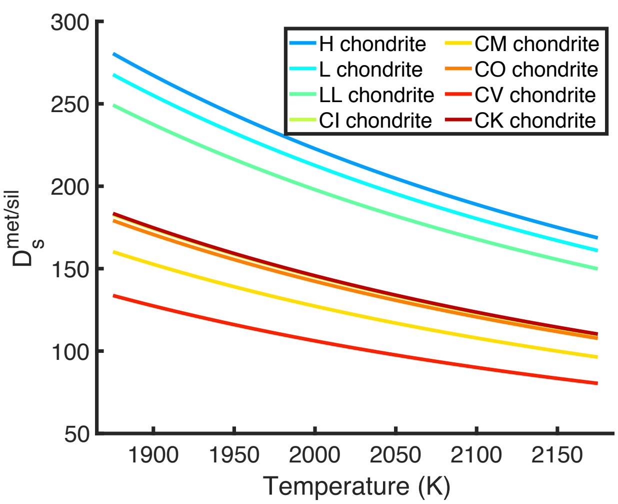

Fig 1. *The change in D_S from 1875 – 2175 K for different chondrites.*

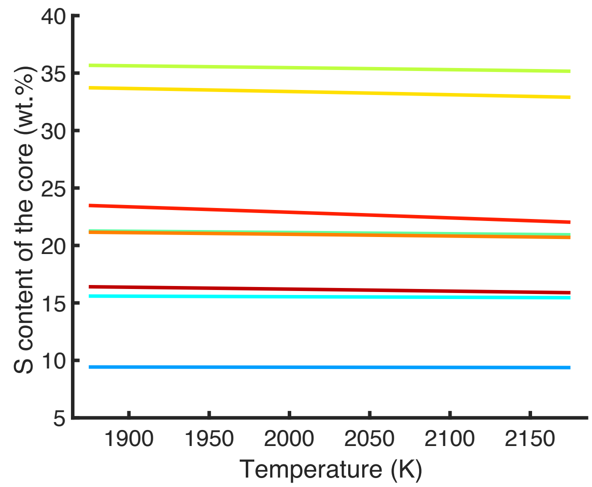

Fig 2. *The sulfur content of the core (wt.%) against temperature during differentiation (K).*

the most troilite and only oxidized iron ($Fe^{2+}O$), resulting in an entirely troilite core.

Discussion: An OC parent body would form a mostly Fe-Ni core, while a CC parent body would form a FeS-rich core. The latter case, though, is geochemically inconsistent with evidence from meteorites. Troilite is only found in nodules and inclusions among meteorites [9]. Also, some iron meteorites thought to come from CC bodies appear to have formed in the presence of sulfur concentrations below those found for CC bodies in this study (Fig. 2) [3, 7]. If CC bodies do form troilite-rich cores, the samples of those cores did not survive the 4.5 Ga years since formation.

Each type of parent body, though, will potentially form an immiscible S-rich liquid [5], though we need to look further into how other light elements alter the immiscibility field of sulfur. Therefore, sulfur could potentially have been removed from the liquid metal in a core, which would explain the lack of sulfur in iron meteorite samples [3]. This suggests that Psyche could have formed a S-rich immiscible fluid after separation from its mantle. If a S-rich fluid formed and made it to Pscyhe's surface, it could be detectable by the spacecraft when it arrives in 2026.

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